Quantum control design by Lyapunov trajectory tracking for dipole and polarizability coupling

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Abstract. We analyse in this paper the Lyapunov trajectory tracking of the Schrödinger equation for a coupling control operator containing both a linear (dipole) and a quadratic (polarizability) term. We show numerically that the contribution of the quadratic part cannot be exploited by standard trajectory tracking tools and propose two improvements: discontinuous feedback and periodic (time-dependent) feedback. For both cases we present theoretical results and support them by numerical illustrations.

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1. Introduction

We consider in this work the evolution of a quantum system with wavefunction $\Psi(t)$ under the external influence of a laser field; the system satisfies the Time Dependent Schrödinger equation (TDSE)

$$i\frac{d}{dt}\Psi(t) = H(t)\Psi(t), \tag{1}$$

with $H(t)$ a Hermitian operator; the control is realized by selecting a convenient laser intensity $u(t)$. When the laser is shut off $H(t)$ is the internal Hamiltonian of the system, denoted H_0; when the laser is present $H(t)$ is the sum of H_0 and additional terms that describe the interaction of the system with the laser field. The first order term is the dipole coupling [30] of the form $u(t)H_1$; in the limit of small laser intensities this term may be enough to adequately describe the interaction.

However, situations exist where the dipole coupling does not have enough influence on the system to reach the control goal; the goal may become accessible only after adding a polarizability term $u^2(t)H_2$ in the expansion of $H(t)$ (see e.g. [13, 14] and related works); to make effective use of this term one needs higher laser intensities $u(t)$.

The focus of the paper is on practical procedures to find suitable control fields $u(t)$ for the Hamiltonian $H(t) = H_0 + u(t)H_1 + u^2(t)H_2$ by adapting feedback tracking control procedures to this setting. Here and in the following H_0, H_1 and H_2 are $n \times n$ Hermitian matrices with complex coefficients and the control is the laser intensity $u(t) \in \mathbb{R}$.

In what concerns the mere possibility to find a control, we recall that the controllability of the finite dimensional quantum system evolving with equation

$$i\frac{d}{dt}\Psi(t) = (H_0 + u(t)H_1 + u^2(t)H_2)\Psi(t), \tag{2}$$

can be studied via the general accessibility criteria [4, 32] based on Lie brackets; more specific results can be found in [34].

Let us consider for a moment the system with Hamiltonian $H_0 + u(t)H_1 + v(t)H_2$, $v(t)$ being a second control independent of $u(t)$. It can be shown [34] that this system is controllable under the same circumstances as $H_0 + u(t)H_1 + u^2(t)H_2$ i.e. all target states that can be reached with Hamiltonian $H_0 + u(t)H_1 + v(t)H_2$ can also be reached by $H_0 + u(t)H_1 + u^2(t)H_2$ (although obviously the second Hamiltonian is a particular case of the first for $v(t) = u^2(t)$). This rather counter-intuitive result suggests that $u^2(t)$ can be considered, for the purpose of theoretical controllability, as independent of $u(t)$; however, $u^2(t)$ having a particular functional dependence on $u(t)$ will play a role at the level of the numerical procedure to find the control: in general finding the control for $H_0 + u(t)H_1 + u^2(t)H_2$ is more difficult than for $H_0 + u(t)H_1 + v(t)H_2$.

The characterization of the controllability does not provide in general a simple and efficient way for open-loop trajectory generation. Optimal control techniques (cf., [23] and [30] and the references herein) provide a first set of methods. A different approach consists in using feedback to generate trajectories and open-loop steering control [5, 19, 22]. More recent results can be found in [27] for decoupling techniques, in [3, 15, 17, 23, 31, 35, 36] for Lyapunov-based techniques and in [1, 7, 28] for factorizations techniques of the unitary group.

In order to study feedback control of systems with Hamiltonian $H(t) = H_0 + u(t)H_1 + u^2(t)H_2$ we adapt the analysis [20, 24], initially proposed for bilinear quantum systems $H_0 + u(t)H_1$. In the previous work it has been shown that the success of the feedback control depends on whether there exists (non-zero) direct coupling, through H_1, between the target state and **all** other eigenstates. When H_1 has the same property for $H(t) = H_0 + u(t)H_1 + u^2(t)H_2$ we show that same feedback formulas hold. However we argued that the polarizability term $u^2(t)H_2$ is added when dipole $u(t)H_1$ is not enough to control the system; consequently the most interesting question is what happens when some of the (direct) coupling is realized by H_2 instead of H_1. We show that the previous feedback formulas do not hold any more and we propose two alternatives. Our method is valid to track any eigenstate trajectory of a Schrödinger equation (2) when the Hamiltonian includes a second order coupling operator.

The balance of the paper is as follows: in Section 2 we introduce the main notations and the Lyapunov tracking feedback for a particular case. Section 3 contains the presentation of two types of feedback: discontinuous and time-dependent (periodic) forcing, that can be applied for all types of second order coupling operators. Both sections present theoretical results on the convergence illustrated by numerical simulations. Concluding remarks are presented in Section 4.

2. Tracking feedback design

2.1. Dynamics and global phase

We consider a n-level quantum system evolving under the equation (2). The wave function $\Psi = (\Psi_j)_{j=1}^n$ is a vector in $\mathbb{C}^n$, verifying $\sum_{j=1}^n |\Psi_j|^2 = 1$, thus it lives on the unit sphere $\mathbb{S}^{2n-1}$ of $\mathbb{C}^n$. Physically, Ψ and $e^{i\theta(t)}\Psi$ describe the same physical state for any global phase $\theta(t) \in \mathbb{R}$, i.e. Ψ_1 and Ψ_2 are identified when exists $\theta(t) \in \mathbb{R}$ such that $\Psi_1 = \exp(i\theta(t))\Psi_2$. To take into account such non trivial geometry we add a second control ω corresponding to $\dot{\theta}$ (see also [24]). Thus we consider the following control system

$$i\frac{d}{dt}\Psi(t) = (H_0 + u(t)H_1 + u^2(t)H_2 + \omega(t))\Psi(t), \tag{3}$$

where $\omega \in \mathbb{R}$ is a new control playing the role of a gauge degree of freedom. We can choose it arbitrarily without changing the physical quantities attached to Ψ. With such additional fictitious control ω, we will assume in the sequel that the state space is $\mathbb{S}^{2n-1}$ and the dynamics given by (3) admits two independent controls u and ω.

2.2. Lyapunov control design

Take a reference trajectory $t \mapsto (\Psi_r(t), u_r(t), \omega_r(t))$, i.e., a smooth solution of (3):

$$i\frac{d}{dt}\Psi_r = (H_0 + u_r H_1 + u_r^2 H_2 + \omega_r)\Psi_r.$$

We introduce the following time varying function $V(\Psi, t)$:

$$V(\Psi) = \langle \Psi - \Psi_r | \Psi - \Psi_r \rangle = \|\Psi - \Psi_r\|^2 \tag{4}$$

where $\langle . | . \rangle$ denotes the Hermitian product. The fonction V is nonnegative for all $t > 0$ and all $\Psi \in \mathbb{S}^{2n-1}$ and vanishes when $\Psi = \Psi_r$, such a V is called a Lyapunov function. The derivative of V is given by:

$$\begin{aligned}\frac{dV}{dt} &= 2(u - u_r) Im(\langle H_1 \Psi(t) | \Psi_r \rangle) \\ &+ 2(u^2 - u_r^2) Im(\langle H_2 \Psi(t) | \Psi_r \rangle) \\ &+ 2(\omega - \omega_r) Im(\langle \Psi(t) \mid \Psi_r \rangle)\end{aligned} \tag{5}$$

where Im denotes the imaginary part.
For convenience we denote: $I_1 = Im(\langle H_1 \Psi(t) | \Psi_r \rangle)$ and $I_2 = Im(\langle H_2 \Psi(t) | \Psi_r \rangle)$. Note that if, for example, one takes

$$\begin{cases} u = u_r(t) - k(I_1 + 2u_r I_2)/(1 + kI_2) \\ \omega = \omega_r(t) - cIm(\langle \Psi(t) \mid \Psi_r \rangle), \end{cases} \tag{6}$$

with k and c strictly positive parameters, one gets

$$dV/dt = -\frac{2}{k}(u - u_r)^2 - 2c(Im(\langle \Psi(t) \mid \Psi_r \rangle))^2 \leq 0,$$

and thus V is nonincreasing.

Remark 2.1 *In order for the denominator $1 + kI_2$ in Eqn. (6) to be non-zero one notes that $|I_2| \leq |\langle H_2 \Psi(t) | \Psi_r \rangle| \leq \|H_2\|$; therefore $1 + kI_2 > 0$ as soon as $k < \frac{1}{\|H_2\|}$. From now on, unless specified otherwise, this condition will be supposed satisfied.*

Let us focus on the important case when the reference trajectory corresponds to an equilibrium: $u_r = 0$, $\omega_r = -\lambda$ and $\Psi_r = \phi$ where ϕ is an eigenvector of H_0 associated to the eigenvalue $\lambda \in \mathbb{R}$ ($H_0\phi = \lambda\phi$, $\|\phi\| = 1$). We obtain:

$$I_1 = Im(\langle H_1 \Psi(t) | \phi), I_2 = Im(\langle H_2 \Psi(t) | \phi). \tag{7}$$

Then (6) becomes a static-state feedback:

$$\begin{cases} u = -kI_1/(1 + kI_2) \\ \omega = -\lambda - cIm(\langle \Psi(t) \mid \phi \rangle). \end{cases} \tag{8}$$

Denote by λ_j, with $j = 1, ..., N$ the eigenvalues of the matrix H_0. Let $\phi_1, \ldots, \phi_n$ be an orthogonal system of corresponding eigenvectors.

We say that H_0 has non-degenerate spectrum if for all $j \neq l$, $j, l = 1, ..., n$, $\lambda_j \neq \lambda_l$.

Although V being nonincreasing is a very important property, this is not enough to ensure that the target state ϕ is reached asymptotically. The following theoretical result for the feedback (8) explains when convergence to target state holds:

Theorem 2.1 *Consider* (3) *with* $\Psi \in \mathbb{S}^{2n-1}$ *and an eigenstate* $\phi \in \mathbb{S}^{2n-1}$ *of* H_0 *associated to the eigenvalue* λ. *Take the static feedback* (8) *with* $c > 0$, $k < \frac{1}{\|H_2\|}$ *and suppose that the spectrum of* H_0 *is non-degenerate. Then the two following propositions are true:*

(i) The limit set of the closed loop system (3) *is in the intersection of* $\mathbb{S}^{2n-1}$ *with the vector space* $E = \mathbb{R}\phi \bigcup_\alpha \mathbb{C}\phi_\alpha$ *where* ϕ_α *is any eigenvector of* H_0 *not co-linear to* ϕ *such that* $\langle \phi_\alpha | H_1 \phi \rangle = 0$.

(ii) If $E = \mathbb{R}\phi$, *the limit set is a subset of* $\{\phi, -\phi\}$.

The proof follows the same ideas as in [24] and it can be found in [16].

Remark 2.2 *The theorem above shows that tracking to* ϕ *works when all eigenstates of* H_0, $\phi_2, ...\phi_n$, *other than* ϕ *are coupled to* ϕ *by* H_1. *However we do not know what happens when some of the coupling are realized by* H_2 *instead (the theorem does not apply but the system is still controllable cf. [34]). We analyze such a case in Section 3. Note that, as pointed out in the Introduction, one uses the model* $H_0 + u(t)H_1 + u^2(t)H_2$ *precisely in the cases when* H_1 *coupling is not enough to control (otherwise taking low laser intensities* $u(t)$ *make* $H_0 + u(t)H_1$ *effective Hamiltonian instead of* $H_0 + u(t)H_1 + u^2(t)H_2$ *and* H_2 *is not longer used to model the system).*

2.3. Examples and simulations

In order to solve (3), we use the following numerical scheme:

$$\psi((m+1)\Delta t) = e^{-i\Delta t(H_0 + u(m\Delta t)H_1 + u^2(m\Delta t)H_2) + \omega(m\Delta t))}\psi(m\Delta t), \tag{9}$$

where m is the index of the time step, $\Delta t = T/M$ is the discretization time step, and M is the total number of time steps. Numerical simulations have been performed for a three-dimensional test system with H_0, H_1 and H_2 given by:

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{3}{2} \end{pmatrix}, \; H_1 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}, \; H_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{10}$$

In this case the wave function is $\Psi = (\Psi_1, \Psi_2, \Psi_3)^T$. We use the Lyapunov control (8) in order to reach the first eigenstate $\phi = (1, 0, 0)$ of energy $\lambda = 0$, at the final time T.

Remark 2.3 *We note that the conditions of Theorem* 2.1 *are fulfilled since:* $\langle \phi_2 | H_1 \phi \rangle \neq 0$ *and* $\langle \phi_3 | H_1 \phi \rangle \neq 0$. *In addition* $\|H_2\| = 1$.

In Figure 1 we plot the evolution of $V = V(\Psi) = \langle \Psi - \phi | \Psi - \phi \rangle$ and u, corresponding to system defined by (10) with feedback (8). We can remark a fast convergence of the Lyapunov function V towards zero, that implies the convergence of Ψ towards $\phi = (1, 0, 0)$. The target goal is achieved with high accuracy at $T = 100$.

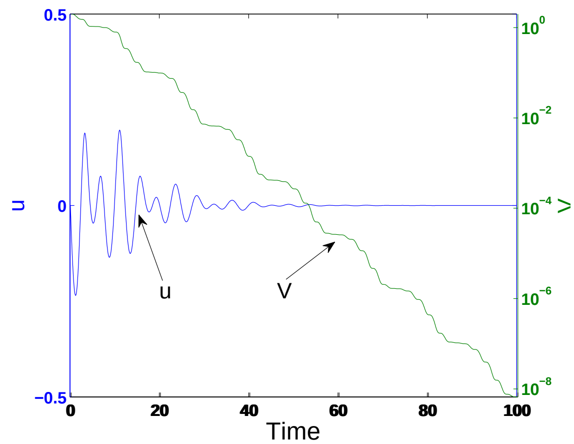

Figure 1. Evolution of the Lyapunov function $V(\Psi)$ (blue line) and control u (green line); initial condition $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (10) with feedback (8). We take $k = 0.2, c = 0.8$.

We consider another three-dimensional test system with H_0, H_1 and H_2 given by:

$$H_0 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{3}{2} \end{pmatrix}, \ H_1 = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \ H_2 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}. \tag{11}$$

In this case the wave function is $\Psi = (\Psi_1, \Psi_2, \Psi_3)^T$. We use the previous Lyapunov control in order to reach the first eigenstate $\phi = (1, 0, 0)$ of energy $\lambda = 0$, at the final time T.

Simulations of Figure 2 start with $(0, 1/\sqrt{2}, 1/\sqrt{2})$ as initial condition for Ψ. Such a feedback reduces the distance to the first state but does not ensure its convergence to $\phi = (1, 0, 0)$ (the Lyapunov function $V(\Psi)$, does not reach the value zero, but stalls at $V = 10^{-0.1}$.) This is not due to a lack of controllability. This system is controllable since the Lie algebra spanned by H_0/i, H_1/i and H_2/i coincides with $u(3)$ (see [24]). As explained in Remark 2.2, such convergence deficiency comes from the fact that operator H_1 couples ϕ only with the state ϕ_2. We plot the evolution of $V(\Psi)$, u, I_1 and I_2, corresponding to system defined by (11) with feedback (8), in Figure 2 and Figure 3.

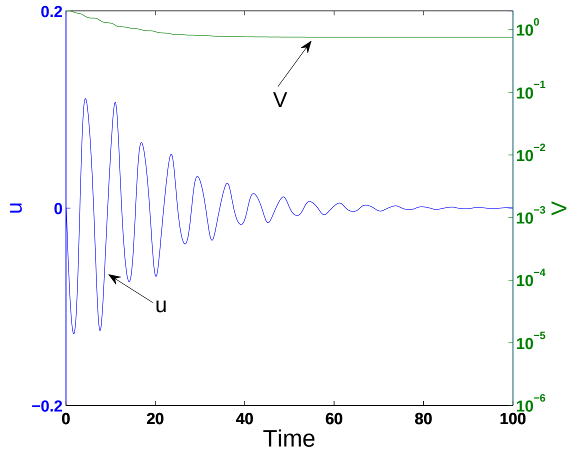

Figure 2. Evolution of the Lyapunov function $V(\Psi)$ (blue line) and control u (green line); initial condition $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (11) with feedback (8). The feedback (8) fails to reach the target, V stalls at $V = 10^{-0.1}$. We take $k = 0.2, c = 0.8$.

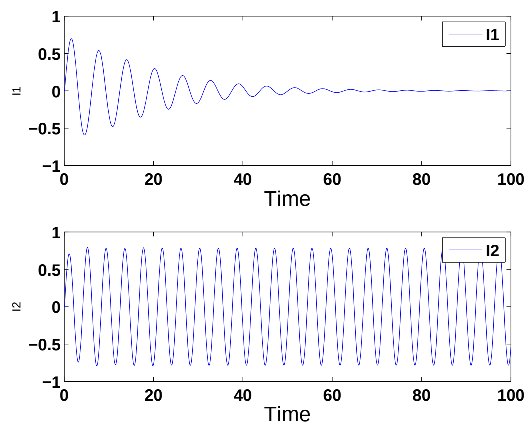

Figure 3. Time evolution of I_1 and I_2; system defined by (11) with feedback (8). We note that I_1 converges to zero. Contrary to I_1, I_2 does not converge to zero.

3. Discontinuous and periodic feedback

In order to stabilize the system when formulas (8) are ineffective, we propose two methods. The first one is to use a special discontinuous feedback ([2, 6, 12, 26], as well as [10, Section 11.4] and the references therein). The second approach is through periodic time dependent feedback ([8, 9] as well as [10, Sections 11.2 and 12.4] and the references therein).

3.1. Discontinuous feedback

For the case of discontinuous feedback we consider the regions: $A = \{|I_1| < \delta \text{ and } \mathrm{I}_2 < -\sqrt{\delta}\}$, $B = \{|I_1| < \delta \text{ and } \mathrm{I}_2 > \sqrt{\delta}\}$, $C = \{|I_1| > \delta/2 \; or \; |I_2| < 2\sqrt{\delta}\}$. Note that A, B, C are open sets; the regions A, C, respectively B, C are overlapping. For $k_1, k_2, c, \delta > 0$ we define the control as follows:

$$u(I_1, I_2) = \begin{cases} k_1 I_2, \; in \; A \setminus C \\ 0, \quad in \; B \setminus C \\ -k_2 I_1/(1 + k_2 I_2), \; in \; C \setminus (A \cup B) \\ for \; A \cap C \; and \; A \cap B \; see \; below, \end{cases} \tag{12}$$

$$\omega = -\lambda - c Im(\langle \Psi(t) \mid \phi \rangle).$$

The definition of $u(I_1, I_2)$ on $A \cap C$ is either $u(I_1, I_2) = k_1 I_2$ (i.e. formula for set A) or $u(I_1, I_2) = -k_2 I_1/(1+k_2 I_2)$ (i.e. formula for set C) is such a way to ensure continuity (with respect to time) of the feedback $u(I_1, I_2)$. Remark that a discontinuity may appear when reaching the border ∂C of C situated in the interior of A (here the formula used is always $u(I_1, I_2) = k_1 I_2$). Same considerations apply for $A \cap B$ (continuity).

We define the propagator $S_1 \Psi_0$ by solving the feedback equation such that: if the initial state $\Psi_0 \in A \cap C$, we initiate with the feedback corresponding to C and if the initial state $\Psi_0 \in B \cap C$, we initiate also with the feedback corresponding to C. We define also the propagator $S_2 \Psi_0$ by solving the feedback equation such that : if the initial state $\Psi_0 \in A \cap C$, we initiate with the feedback corresponding to A and if the initial state $\Psi_0 \in B \cap C$, we initiate also with the feedback corresponding to B. We continue with the feedback for the given region until reaching the boundary of this one, then we switch to the feedback corresponding to the next overlapping region. Observe that neither S_1 nor S_2 define a classical dynamical system, that is the semigroup property is lost. One has instead:

$$S_1(t + s)\Psi_0 = S_1(t) S_1(s) \Psi_0 \text{ or } \mathrm{S}_1(\mathrm{t}+\mathrm{s})\Psi_0 = \mathrm{S}_2(\mathrm{t})\mathrm{S}_1(\mathrm{s})\Psi_0. \tag{13}$$

The propagators $S_1(t)\Psi_0$ and $S_2(t)\Psi_0$ are solutions in the sense of Carathéodory for the feedback controlled system and depend continuously on the initial data. These solutions are well defined locally and they are globally defined on $[0, \infty[$; this follows from the fact that intervals of time between switching moments are bounded from bellow by a strictly positive constant.

We now turn to the question of the negativity of dV/dt.

(i) when $u(I_1, I_2) = -k_2 I_1/(1 + k_2 I_2)$, i.e. in the region $C \setminus (A \cup B)$ and possibly $A \cap C$ and $B \cap C$, we obtain the following constraint on k_2 (cf. also Remark 2.1): $k_2 < \frac{1}{\|H_2\|}$; with this provision $dV/dt < 0$ in this region.

(ii) when $u = 0$, i.e. in the region $B \setminus C$ and possibly $C \cap B$: $dV/dt = 0$

(iii) when $u(I_1, I_2) = k_1 I_2$, i.e. in the region $A \setminus C$ and possibly $A \cap C$: $dV/dt = u I_1 + u^2 I_2 = u(I_1 + u I_2) = k_1 I_2 (I_1 + k_1 (I_2)^2)$. On the set A the term I_2 is less than $-\sqrt{\delta}$ and thus $k_1 I_2$ is strictly negative. From the definition of A the term $I_1 + k_1(I_2)^2$ is lower bounded by $-\delta + k_1\delta$; thus for $k_1 > 1$ the term $I_1 + k_1(I_2)^2$ is strictly positive thus $dV/dt < 0$.

Therefore $k_1 > 1$ and $k_2 < \frac{1}{\|H_2\|}$ imply $dV/dt \leq 0$ with $dV/dt = 0$ only when $u(I_1, I_2) = 0$. Moreover one has the following convergence result for the feedback (12) (see also [11]).

Theorem 3.1 *Consider* (3) *with* $\Psi \in \mathbb{S}^{2n-1}_{\mathbb{C}}$ *and an eigenstate* $\phi \in \mathbb{S}^{2n-1}_{\mathbb{C}}$ *of* H_0 *associated to the eigenvalue* λ. *Take the feedback* (12) *with* $k_1 > 1$, $k_2 < \frac{1}{\|H_2\|}$ *and* $c, \delta > 0$. *If* H_0 *is not degenerate and for every* k *with* $\phi_k \neq \phi$ *either* $\langle \phi_k | H_1 \phi \rangle \neq 0$ *or* $\langle \phi_k | H_2 \phi \rangle \neq 0$ *then the limit set of* $\Psi(t)$ *reduces to a solution of the uncontrolled system, with* $|I_1| < \delta$, $|I_2| \leq C\sqrt{\delta}$ *with a constant* C *depending only on* H_0.

Proof of Theorem 3.1. Up to a shift on ω and H_0, we can assume that $\lambda = 0$.

Trajectories corresponding to the propagator S_1 are relatively compact so the limit points at infinity form a limit set Ω_δ which is compact and connected.

On the limit set Ω_δ, V is constant and from the relation (13), Ω_δ is invariant either to S_1 or to S_2, that is if $\Psi_1 \in \Omega_\delta$ then $S_1(t)\Psi_1 \in \Omega_\delta, t > 0$ or $S_2(t)\Psi_1 \in \Omega_\delta, t > 0$.

The limit set Ω_δ is a union of trajectories of equation (3) corresponding either to the propagator S_1 or to the propagator S_2, along this trajectories V is constant, so $dV/dt = 0$ where V is defined by (4). The equation $dV/dt = 0$ means that:

$$u(I_1 + uI_2) = 0, \tag{14}$$

$$Im\langle \Psi, \phi \rangle = 0. \tag{15}$$

Since u is defined by (12) it follows that the limit set, Ω_δ, consists in fact of trajectories of the uncontrolled system:

$$i\frac{d}{dt}\Psi = H_0\Psi. \tag{16}$$

with the solutions of the form:

$$\Psi = \sum_{j=1}^{n} b_j e^{-i\lambda_j t}\phi_j. \tag{17}$$

For the same reasons as above we obtain that the limit set Ω_δ is characterized by:

$$\Omega_\delta \subset \{I_1 = 0 \textit{ and } |I_2| < 2\sqrt{\delta}\} \cup \{|I_1| < \delta \textit{ and } I_2 > \sqrt{\delta}\}. \tag{18}$$

From relation (18) we have that on the limit set $|I_1| < \delta$. We substitute (17) in (15) and we have:

$$Im\langle \Psi, \phi \rangle = Im(b_1)\langle \phi, \phi \rangle + \sum_{j=2}^{n} Im(b_j \langle \phi_j, \phi \rangle e^{-i\lambda_j t}) = 0. \tag{19}$$

We obtain $Im(b_1) = 0$. We denote by $J_1 = \{j | j \neq 1, \langle H_1\phi_j | \phi \rangle) \neq 0\}$ and $J_2 = \{j | j \neq 1, \langle H_2\phi_j | \phi \rangle) \neq 0\}$. We have by the hypothesis that $J_1 \cup J_2 = \{2, 3, \ldots, n\}$.

We substitute (17) in (7), and we obtain:

$$I_1 = Im(b_1)\langle H_1\phi,\phi\rangle + \sum_{j\in J_1} Im(b_j\langle H_1\phi_j,\phi\rangle e^{-i\lambda_j t}), \tag{20}$$

$$I_2 = Im(b_1)\langle H_2\phi,\phi\rangle + \sum_{j\in J_2} Im(b_j\langle H_2\phi_j,\phi\rangle e^{-i\lambda_j t}). \tag{21}$$

Since $Im(b_1) = 0$ we have:

$$I_2 = \sum_{j\in J_2} Im(b_j\langle H_2\phi_j,\phi\rangle e^{-i\lambda_j t}) = \sum_{j\in J_2} B_j \sin(\lambda_j t + \theta_j). \tag{22}$$

where the coefficients $B_j = 0$ if and only if $b_j = 0$, $j \in J_2$. We define $M = \sup(I_2)$ and $m = \inf(I_2)$. There exists $C > 0$ independent of B_j and θ_j such that $M \leqslant -Cm$. Since on the limit set Ω_δ, $I_2 \geqslant -2\sqrt{\delta}$ it is easy to verify that $|I_2| \leqslant C\sqrt{\delta}$.

Remark 3.1 *In order to make the conclusion of the theorem more precise note that if* Ψ_δ *is a trajectory of* (16) *belonging to* Ω_δ*, then when* δ *converges to zero,* $\Psi_\delta \to \phi$ *, if the initial state is different of* $-\phi$*. Accordingly, when* I_1, I_2 *are small* $V(\Psi)$ *will also be small and the system is close to the target state.*

The practical question is then how small should one choose δ*. A way to circumvent this question is to consider not a constant value* δ *but one that decreases over time; this way the problem will take itself care of finding the good value of* δ *for a given precision. Numerical results (not shown here) confirm the interest of this approach.*

Remark 3.2 *An important ingredient of the proof is finding the limit sets of the evolution, which itself depends very much on the choice of the sets* A, B, C *and of the controls* u*. The general rationale behind these choice are to modify formula (8) minimally in order to have good properties of* Ω_δ*.*

3.1.1. Examples for non-degenerate cases. We take the system (11) and apply the discontinuous feedback (12). Simulations of Figure 4 describe the evolution of the Lyapunov function $V(\Psi)$ and control u, for the initial state $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$. In this case: $k_1 = 1.1$, $k_2 = c = 0.8$ and $\delta = 1.e-4$.

It appears that this feedback is quite efficient for system (11). We present the evolution of I_1 and I_2 corresponding to system defined by (11), with feedback (12), in Figure 5.

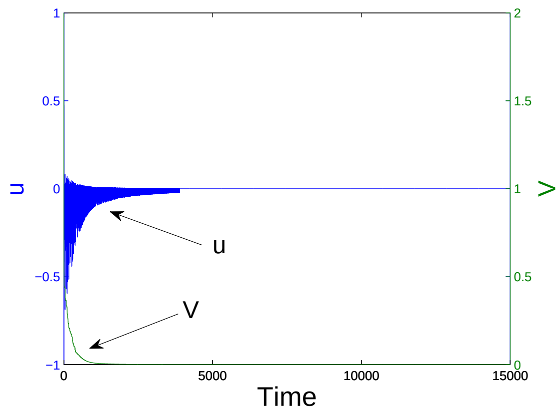

Figure 4. Evolution of the Lyapunov function $V(\Psi)$(blue line) and control u (green line); initial condition: $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (11) with feedback (12)($k_1 = 1.1$, $k_2 = c = 0.8$, $\delta = 1.e - 4.$).

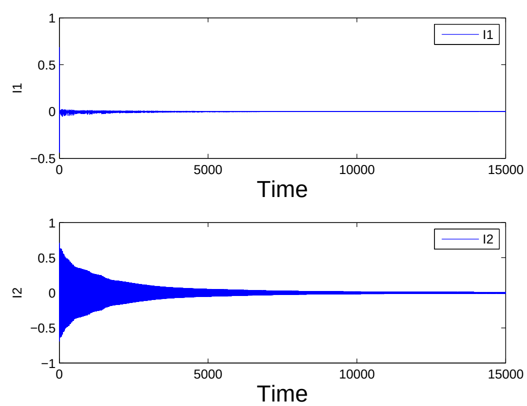

Figure 5. Time evolution of I_1 and I_2; system defined by (11) with feedback (12); $|I_1| < \delta$ and $|I_2| \leqslant C\delta$.

We consider next the five-dimensional system (see [33]) defined by

$$H_0 = \begin{pmatrix} 1.0 & 0 & 0 & 0 & 0 \\ 0 & 1.2 & 0 & 0 & 0 \\ 0 & 0 & 1.3 & 0 & 0 \\ 0 & 0 & 0 & 1.4 & 0 \\ 0 & 0 & 0 & 0 & 2.15 \end{pmatrix}, H_1 = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \end{pmatrix}, H_2 = \begin{pmatrix} 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 \end{pmatrix} \tag{23}$$

We use the previous Lyapunov control in order to reach the first eigenstate $\phi = (1, 0, 0, 0, 0, 0)$ of energy $\lambda = 1$, at the final time T. Note that here $\|H_2\| = 1$.
Simulations of Figure 6 describe the evolution of the Lyapunov function $V(\Psi)$ and control u, for the initial state $\Psi(t = 0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$. We take $k_1 = 1.1$, $k_2 = c = 0.8$ and $\delta = 1.e - 4$.

We present the evolution of I_1 and I_2 corresponding to system defined by (23), with feedback (12), in Figure 7.

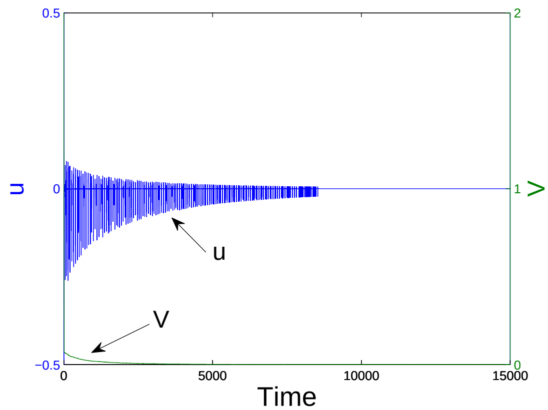

Figure 6. Evolution of the Lyapunov function $V(\Psi)$(blue line) and control u (green line); initial condition: $\Psi(t=0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$; system defined by (23) with feedback (12) ($k_1 = 1.1, k_2 = c = 0.8$, $\delta = 10^{-4}$).

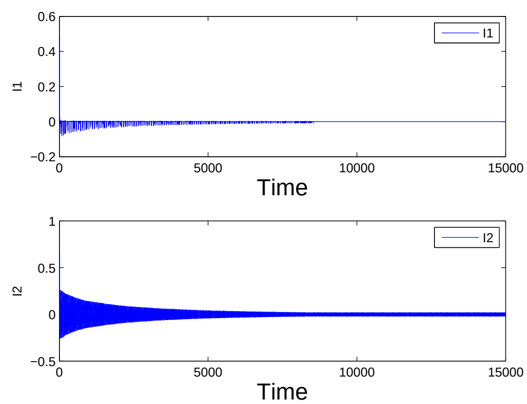

Figure 7. Time evolution of I_1 and I_2; system defined by (23) with feedback (12); $|I_1| < \delta$ and $|I_2| \leqslant C\delta$.

3.1.2. Examples for degenerate cases. There are various situations where the condition of non degeneracy of the Hamiltonian H_0, present in Theorem 2.1 and Theorem 3.1 is non fulfilled. One such example is given below (see [18, 25]):

$$H_0 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0.04556 & 0 & 0 \\ 0 & 0 & 0.095683 & 0 \\ 0 & 0 & 0 & 0.095683 \end{pmatrix}, H_1 = \begin{pmatrix} 0 & 1 & 1 & -1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}, H_2 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix} \quad (24)$$

The internal Hamiltonian H_0 is degenerate since $\lambda_3 = \lambda_4 = 0.095683$, but it can be stabilized using the discontinuous feedback defined by (12). Here $\|H_2\| = 1$.

Simulations of Figure 8 describe the evolution of the Lyapunov function $V(\Psi)$ and control u, system defined by (24) starting from the initial state $\Psi(t=0) = (0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$.

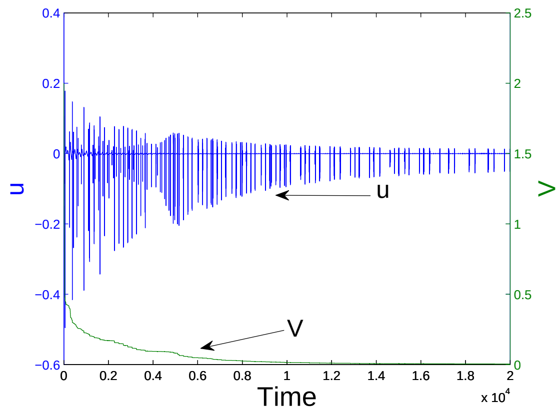

Figure 8. Evolution of the Lyapunov function $V(\Psi)$ (blue line) and control u (green line); initial condition $\Psi(t = 0) = (0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$; system defined by (24) with feedback (12) ($k_1 = 1.1$, $k_2 = c = 0.8$, $\delta = 1.e - 4$).

This positive result for degenerate system shows that the theoretical results are sufficient but not necessary; however the approach may fail in some particular degenerate cases.This is consistent with the literature on quantum control that shows that degenerate cases have special structure (starting even with controllability criteria).

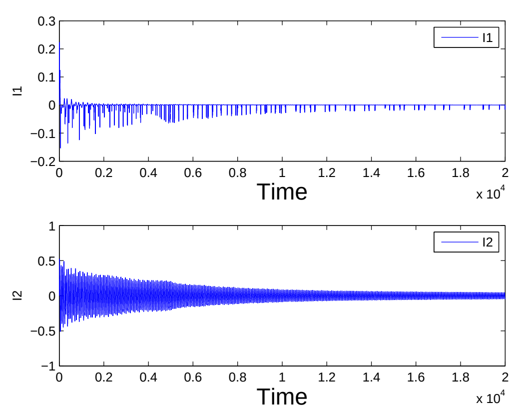

Figure 9. Time evolution of I_1 and I_2; system defined by (24) with feedback (12).

3.2. Periodic feedback

Although the discontinuous feedback (12) gives satisfactory results in terms of the control quality, the fact that it is discontinuous motivates trying to find additional procedures. To this end we introduce in this section a periodic, time dependent, feedback $u = u(t, \Psi)$ stabilizing (3) to the ground state ϕ. The idea is to use a highly oscillatory field component whose linear contribution averages to zero while the quadratic part averages to a constant; then we compare the asymptotic behavior of the system with the behavior of the averaged system. We recall that we are in the case when the reference trajectory corresponds to an equilibrium.

We consider the following time dependent feedback:

$$u(t,\Psi) = \alpha(\Psi) + \beta(\Psi)\sin(t/\varepsilon). \tag{25}$$

We substitute (25) in (3) and we obtain the system:

$$\begin{aligned} i\frac{d}{dt}\Psi(t) = \Big(&H_0 + \alpha(\Psi)H_1 + \beta(\Psi)\sin(t/\varepsilon)H_1 \\ &+ \alpha^2(\Psi)H_2 + 2\alpha(\Psi)\beta(\Psi)\sin(t/\varepsilon)H_2 \\ &+ \beta^2(\Psi)\sin^2(t/\varepsilon)H_2 + \omega(t)\Big)\Psi(t). \end{aligned} \tag{26}$$

The averaged system is given by (see [21] pages 402-410):

$$i\frac{d}{dt}\Psi_{av} = (H_0 + \alpha H_1 + (\alpha^2 + \frac{1}{2}\beta^2)H_2 + \omega)\Psi_{av}. \tag{27}$$

We identify the coefficients α and β such that the averaged system is asymptotically stable. We use a Lyapunov technique to stabilize the averaged system (27) around the ground state ϕ. We take again the function V defined by (4), which is nonnegative for all $\Psi \in \mathbb{S}^{2n-1}$ and vanishes when $\Psi = \phi$.

The derivative of V along a trajectory of the averaged system (26) is given by:

$$\begin{aligned} \frac{d}{dt}V(\Psi_{av}(t)) = &2\alpha Im(\langle H_1\Psi_{av}(t)|\phi\rangle) + 2\alpha^2 Im(\langle H_2\Psi_{av}(t)|\phi) \\ &+ \beta^2 Im(\langle H_2\Psi_{av}(t)|\phi\rangle) + 2(\omega+\lambda)Im(\langle\Psi_{av}(t)|\phi\rangle). \end{aligned} \tag{28}$$

We denote: $I_1^{av} = Im(\langle H_1\Psi_{av}(t)|\phi\rangle)$ and $I_2^{av} = Im(\langle H_2\Psi_{av}(t)|\phi\rangle)$. When, for instance, we take:

$$\alpha = -kI_1^{av},\ \beta = (I_2^{av})^-,\ \omega = -\lambda - cIm(\langle\Psi_{av}(t)|\phi\rangle), \tag{29}$$

we obtain:

$$\frac{d}{dt}V(\Psi_{av}(t)) = -2\Big(k(I_1^{av})^2(1-kI_2^{av}) + \frac{((I_2^{av})^-)^3}{2} + cIm^2(\langle\Psi_{av}(t)|\phi\rangle)\Big) \tag{30}$$

and thus $dV/dt \leq 0$, for $c > 0$ and $k < \frac{1}{\|H_2\|}$ (cf. Remark 2.1), *i.e.* V is nonincreasing along the trajectories of the averaged system. In particular ϕ is a stable point for the averaged system, i.e. such that

$$\forall\delta > 0,\ \exists\delta' > 0 \text{ such that } (|\Psi_{av}(0) - \phi| < \delta') \Rightarrow (|\Psi_{av}(t) - \phi| < \delta,\ \forall\ t \in [0, +\infty)). \tag{31}$$

We have the following asymptotic stability result:

Theorem 3.2 *Under the hypotheses:*

(i) $\lambda_j \neq \lambda_l$ *for* $j \neq l$,

(ii) for any $j = 2, .., n$: $\langle H_1\phi_j|\phi\rangle \neq 0$ *or* $\langle H_2\phi_j|\phi\rangle \neq 0$,

the averaged system (27) *is globally asymptotically stable on* $\mathbb{S}^{2n-1} \setminus \{-\phi\}$ *in the sense (recall* (31)*) that every solution* Ψ_{av} *of* (27) *with an initial state other than* $-\phi$ *tends to* ϕ *as* t *tends to* $+\infty$.

Proof of Theorem 3.2 Up to a shift on ω and H_0, we may assume that $\lambda = 0$. LaSalle's principle (see, e.g., [21, Theorem 3.4, page 115]) says that the trajectories of the system (27) converge to the largest invariant set contained in $dV_{av}/dt = 0$. The equation $dV/dt = 0$ means that:

$$I_1^{av} = 0,\ (I_2^{av})^- = 0,\ Im(\langle\Psi_{av}(t)|\phi\rangle) = 0, \tag{32}$$

and therefore $\alpha = \beta = 0$.

On the Ω-limit set of a trajectory, V is constant. Since the Ω-limit set is invariant under the flow generated by (27) it follows that it consists in fact of trajectories of the uncontrolled system:

$$i\frac{d}{dt}\Psi_{av} = H_0\Psi_{av}. \tag{33}$$

The solutions of (33) have the form:

$$\Psi_{av} = \sum_{j=1}^{n} b_j e^{-i\lambda_j t}\phi_j, \tag{34}$$

We substitute (34) in (32) and we obtain:

$$Im(\langle\Psi_{av}(t)|\phi\rangle) = Im(b_1)\langle\phi,\phi\rangle + \sum_{j=2}^{n} Im(b_j\langle\phi_j,\phi\rangle e^{-i\lambda_j t}), \tag{35}$$

$$I_1^{av} = Im(b_1)\langle H_1\phi,\phi\rangle + \sum_{j\in J_1} Im(b_j\langle H_1\phi_j,\phi\rangle e^{-i\lambda_j t}), \tag{36}$$

$$I_2^{av} = Im(b_1)\langle H_2\phi,\phi\rangle + \sum_{k\in J_2} Im(b_j\langle H_2\phi_j,\phi\rangle e^{-i\lambda_j t}). \tag{37}$$

From equation (32) and (35) we obtain that $Im(b_1) = 0$. Since along the trajectories in Ω, $I_1^{av} \equiv 0$ we obtain $b_j = 0, j \in J_1$. Using $Im(b_1) = 0$ we have:

$$I_2^{av} = \sum_{j\in J_2} Im(b_j\langle H_2\phi_j,\phi\rangle e^{-i\lambda_j t}) = \sum_{j\in J_2} B_j \sin(\lambda_j t + \theta_j), \tag{38}$$

where the coefficients $B_j = 0$ if and only if $b_j = 0$, $j \in J_2$. Since $I_2^{av} \geq 0\,\forall t$, it follows that $I_{av}^2 \equiv 0$. We have thus $b_j = 0, j \neq 1$. We obtain that $\Omega \subset \{\phi, -\phi\}$. This concludes the proof of Theorem 3.2.

Our next theorem shows that our time-varying feedback laws lead to some kind of "practical global asymptotic stability on $\mathbb{S}^{2n-1} \setminus \{-\phi\}$" if $\varepsilon > 0$ is small enough and if the assumptions of Theorem 3.2 hold (see also [11]).

Theorem 3.3 *Let us assume that (i) and (ii) of Theorem 3.2 hold. Let $\mathcal{V}$ be a neighborhood of $-\phi$ and let $\delta \in (0, +\infty)$. Then there exist $T > 0$ and $\epsilon_0 > 0$ such that, for every $\tau > 0$ and for every solution Ψ of (26) with $\epsilon \in (0, \epsilon_0)$ and $\Psi(\tau) \in \mathbb{S}^{2n-1} \setminus \mathcal{V}$,*

$$|\Psi(t) - \phi| < \delta \text{ for every } t \geqslant \tau + T. \tag{39}$$

Proof of Theorem 3.3. The key ingredient is the following classical lemma (see, e.g., [21, pages 415-417] or [29, Section 3.2]).

Lemma 3.1 *Let $T > 0$. There exists C and $\varepsilon_0 > 0$ such that, for every $\tau \in \mathbb{R}$ and for every $\varepsilon \in (0, \varepsilon_0)$, if $\Psi : [\tau, \tau + T] \to \mathbb{S}^{2n-1}$ is a solution of (26) and Ψ_{av} is the solution of the averaged system (27) such that $\Psi_{av}(\tau) = \Psi(\tau)$, then*

$$|\Psi(t) - \Psi_{av}(t)| < C\varepsilon, \ \forall t \in [\tau, \tau + T]\,.$$

Let $\delta_1 > 0$ be such that

$$(|\xi - \phi| < \delta_1) \Rightarrow (\xi \notin \mathcal{V}). \tag{40}$$

By (31), there exists $\delta_2 > 0$ such that, for every solution Ψ_{av} of the averaged system (27),

$$(|\Psi_{av}(0) - \phi| < 2\delta_2) \Rightarrow \left(|\Psi_{av}(t) - \phi| < \frac{\min\{\delta, \delta_1\}}{2} \, \forall t \in [0, +\infty)\right). \tag{41}$$

By Theorem 3.2, there exists $T > 0$ such that, for every solution Ψ_{av} of the averaged system (27),

$$(\Psi_{av}(0) \in \mathbb{S}^{2n-1} \setminus \mathcal{V}) \Rightarrow (|\Psi_{av}(t) - \phi| < \delta_2 \, \forall t \in [T, +\infty)). \tag{42}$$

By Lemma 3.1 and (42), there exists $\epsilon_1 > 0$ such that, for every $\varepsilon \in (0, \varepsilon_1)$, for every $\tau \in \mathbb{R}$ and for every solution Ψ of (26),

$$(\Psi(\tau) \in \mathbb{S}^{2n-1} \setminus \mathcal{V}) \Rightarrow (|\Psi(\tau + T) - \phi| < 2\delta_2). \tag{43}$$

By Lemma 3.1 and (41), there exists $\varepsilon_2 > 0$ such that, for every $\varepsilon \in (0, \varepsilon_2)$, for every $\tau' \in \mathbb{R}$ and for every solution Ψ of (26),

$$(|\Psi(\tau') - \phi| < 2\delta_2) \Rightarrow (|\Psi(\tau' + t) - \phi| < \min\{\delta, \delta_1\} \, \forall t \in [0, T]). \tag{44}$$

Let us check that the conclusion of Theorem 3.3 holds with $\varepsilon_0 = \min\{\varepsilon_1, \varepsilon_2\}$. Let $\varepsilon \in (0, \min\{\varepsilon_1, \varepsilon_2\})$, let $\tau > 0$ and let Ψ be a solution of (26) such that $\Psi(\tau) \in \mathbb{S}^{2n-1} \setminus \mathcal{V}$. By (43),

$$|\Psi(\tau + T) - \phi| < 2\delta_2. \tag{45}$$

From (44) with $\tau' = \tau + T$ and (45), one gets that

$$|\Psi(\tau + t) - \phi| < \min\{\delta, \delta_1\} \leq \delta \, \forall t \in [T, 2T]. \tag{46}$$

From (40) and (46) for $t = T$, one gets that

$$\Psi(\tau + T) \notin \mathcal{V}. \tag{47}$$

Using (47) and applying (46) with $\tau + T$ for the new value of τ, one gets that

$$|\Psi(T + \tau + t) - \phi| < \min\{\delta, \delta_1\} \leq \delta \, \forall t \in [T, 2T].$$

Keeping going, an easy induction argument on the integer m shows that, more generally, for every nonnegative integer m,

$$|\Psi(mT + \tau + t) - \phi| < \min\{\delta, \delta_1\} \leq \delta \, \forall t \in [T, 2T],$$

which implies (39).

3.2.1. Examples for non-degenerate cases. We take the system (11) and apply the periodic feedback (25) with α et β defined by (29). Simulations of Figure 10 describe the evolution of the Lyapunov function $V(\Psi)$ for the initial state $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$.

It appears that the periodic feedback is quite efficient for system (11). See Figure 10.

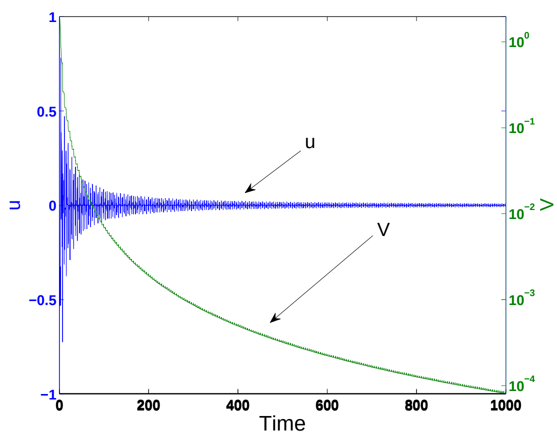

Figure 10. Evolution of the Lyapunov function $V(\Psi)$(blue line) and control u (green line); initial condition: $\Psi(t = 0) = (0, 1/\sqrt{2}, 1/\sqrt{2})$; system defined by (11) with feedback (25). We take $\varepsilon = 1.e - 3$, $k = 0.8, c = 0.5$.

We take the system (23) and apply the periodic feedback (25) with α et β defined by (29). Simulations of Figure 11 describe the evolution of the Lyapunov function $V(\Psi)$ and control u for the initial state $\Psi(t = 0) = (0, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4}, 1/\sqrt{4})$. Agreement with the theoretical results presented above is obtained. See Figure 11.

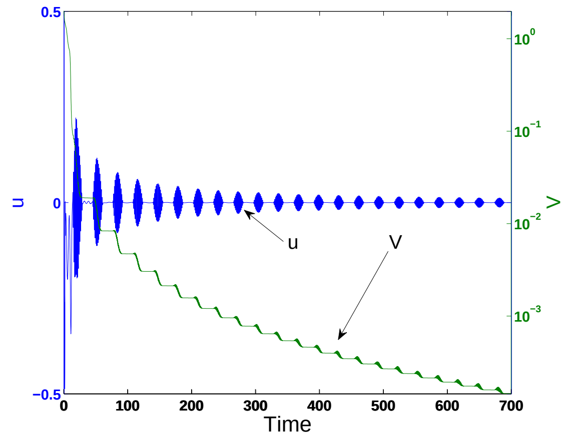

Figure 11. Evolution of the Lyapunov function $V(\Psi)$(blue line) and control u (green line); initial condition: $\Psi(t=0) = (0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$; system defined by (23) with feedback (25). We take $\varepsilon = 1.e-3$, $k = 0.8, c = 0.5$.

3.2.2. Examples for degenerate cases. We take the system defined by (24) and we apply the periodic feedback (25) with α et β defined by (29). Simulations of Figure 12 describe the evolution of the Lyapunov function $V(\Psi)$ and control u, system defined by (24) starting from the initial state $\Psi(t=0) = (0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$. We present the evolution of I_1 and I_2 corresponding to system defined by (24), with feedback (25), in Figure 13.

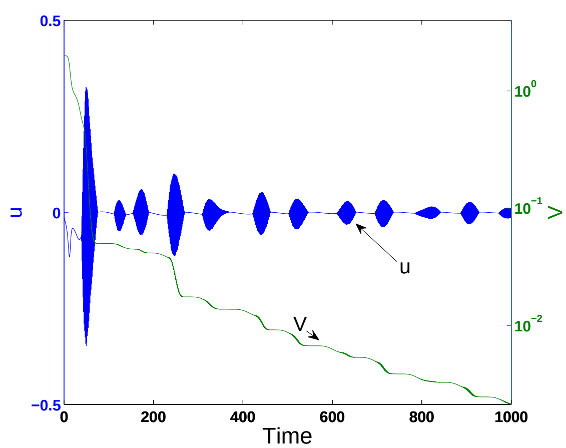

Figure 12. Evolution of the Lyapunov function $V(\Psi)$(blue line) and control u (green line); initial condition $\Psi(t=0) = (0, 1/\sqrt{3}, 1/\sqrt{3}, 1/\sqrt{3})$; system defined by (24) with feedback (25). We take $\varepsilon = 1.e-3$, $k = 0.8, c = 0.5$.

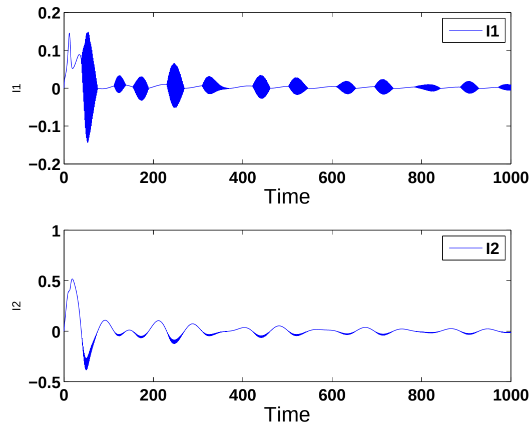

Figure 13. Time evolution of I_1 and I_2; system defined by (24) with feedback (25).

4. Conclusions

We focus in this paper on designing trajectory tracking (feedback) procedures for a control system with polarizability terms $u^2(t)H_2$ present. We find that a straightforward application of the previous results only work for systems that are controllable without the polarizability term. To be able to find a control field that exploit the polarizability coupling we propose two different solutions: the first one is to use a discontinuous feedback with memory terms, the other is to use time-dependent (periodic) forcing. In both cases we present related theoretical results and numerically implement these techniques on prototypical examples. The time-dependent feedback is seen to generally produce smoother controls.

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